IWOMP INTERNATIONAL WORKSHOP 2020

TACC, Austin, Texas - Virtual
21-24 September 2020

A Tale of Four Packages

Jack Dongarra
University of Tennessee
Oak Ridge National Laboratory
University of Manchester

In collaboration with Ahmad Abdelfattah, Mark Gates, Azzam Haidar, Jakub Kurzak, Piotr Luszczek , Stan Tomov, Asim YarKhan, and more at ICL and many more internationally

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Outline for the Talk

- Its about dense linear algebra software and packages
  - LAPACK and ScaLAPACK in the ‘90s & ‘00s
  - PLASMA in the ‘10s
  - MAGMA in the ‘10s
  - SLATE in the ‘20s

DLA Solvers

- We are interested in developing Dense Linear Algebra Solvers
- Retool LAPACK and ScaLAPACK for multicore and hybrid architectures
  - These are two very successful packages
  - They have transitioned to vendors, both hardware and software, which provide optimized versions.

Dense Linear Algebra

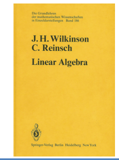
- Common Operations

$$Ax = b; \quad \min_x \| Ax - b \|; \quad Ax = \lambda x$$

- A major source of large dense linear systems is problems involving the solution of boundary integral equations.
  - The price one pays for replacing three dimensions with two is that what started as a sparse problem in $O(n^3)$ variables is replaced by a dense problem in $O(n^2)$.
- Dense systems of linear equations are found in numerous other applications, including:
  - Electronic structures;
  - Maxwell equations;
  - Plasma containment;
  - Airplane wing design;
  - Radar cross-section studies;
  - Flow around ships and other off-shore constructions;
  - Diffusion of solid bodies in a liquid;

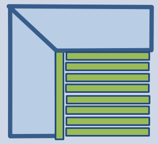
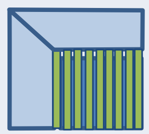
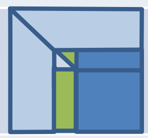
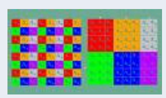
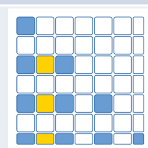
See: **Large Dense Numerical Linear Algebra in 1993: the Parallel Computing Influence,** Alan Edelman, *The International Journal of Supercomputing Applications*. 1993; 7(2):113-128. doi:10.1177/109434209300700203

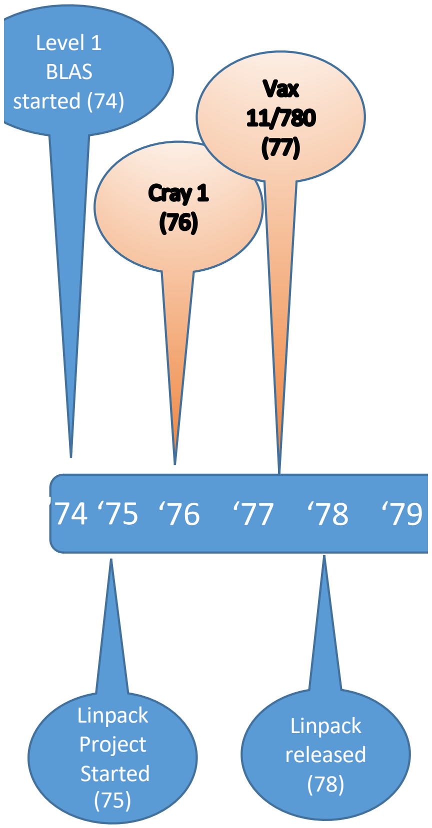
50 Years Evolving SW and Alg Tracking Hardware Developments



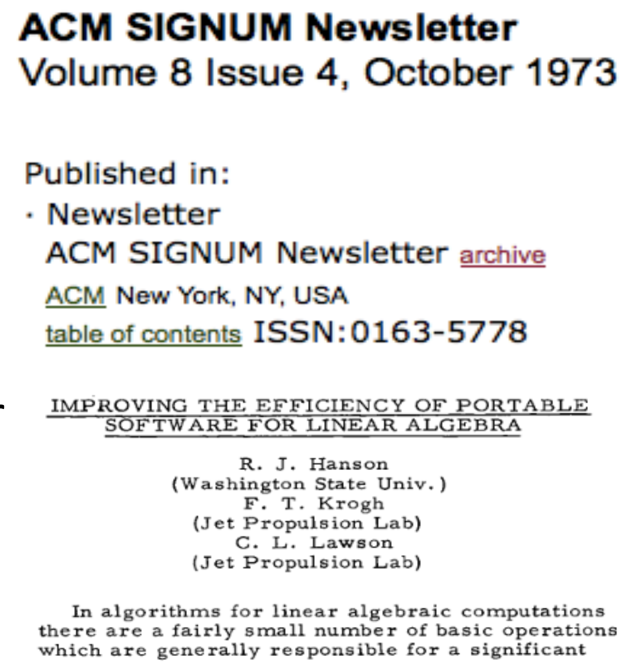
Handbook:
Set the stage and tone

Software/Algorithms follow hardware evolution in time

EISPACK (1970s) (Translation of Algol to F66)	 	Rely on - Fortran, but row oriented
LINPACK (1980s) (Vector operations)	 	Rely on - Level-1 BLAS operations - Column oriented
LAPACK (1990s) (Blocking, cache friendly)	 	Rely on - Level-3 BLAS operations
ScaLAPACK (2000s) (Distributed Memory)	 	Rely on - PBLAS for Message Passing
PLASMA & MAGMA (2010s) New Algorithms (many-core friendly & GPU)		Rely on - DAG/scheduler - block data layout - some extra kernels
SLATE (2020s)		Distributed Memory Rely on C++ - Tasking DAG scheduling - Tiling, but tiles can come from anywhere - Batched Dispatch



- 1974: Effort to standardize Basic Linear Algebra Subprograms
  - Basic LA vector operations
  - Referred to now as Level 1 BLAS
    - Dot product, 2-norm, α*x+y, α*x, etc.
- 1975: LINPACK Project started
  - Effort to produce portable, efficient linear algebra software for dense matrix computations.
- 1976: Vector computers in use for HPC
- 1977: DEC VAX system in common use

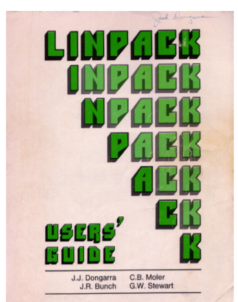

ACM SIGNUM Newsletter
Volume 8 Issue 4, October 1973

Published in:
- Newsletter
  ACM SIGNUM Newsletter archive
  ACM New York, NY, USA
  table of contents ISSN:0163-5778

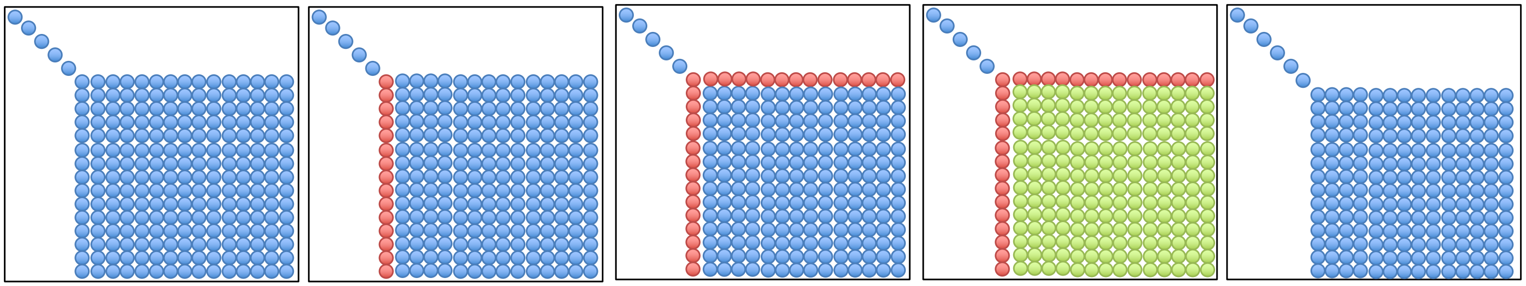
IMPROVING THE EFFICIENCY OF PORTABLE SOFTWARE FOR LINEAR ALGEBRA

R. J. Hanson
(Washington State Univ.)
F. T. Krogh
(Jet Propulsion Lab)
C. L. Lawson
(Jet Propulsion Lab)

In algorithms for linear algebraic computations there are a fairly small number of basic operations which are generally responsible for a significant



The Standard LU Factorization LINPACK
1970's HPC of the Day: Vector Architecture



Factor column with Level 1 BLAS

Divide by Pivot row

Schur complement update (Rank 1 update)

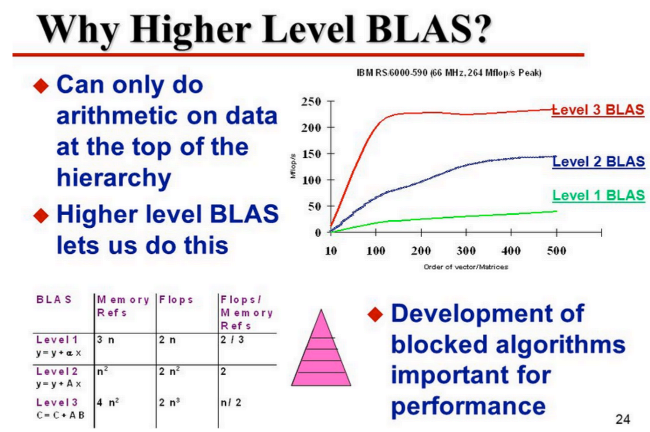
Next Step

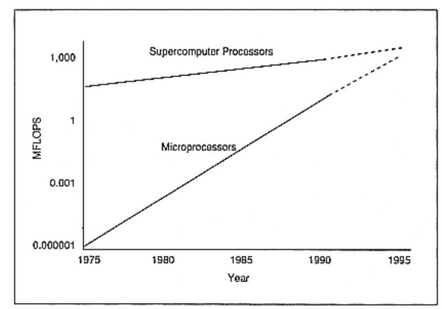
Main points

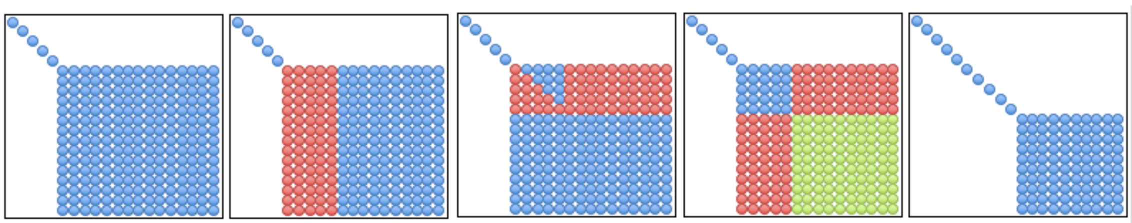
- Fortran was the language, implied column orientation
- Factorization column (zero) mostly sequential due to memory bottleneck
- Level 1 BLAS
- Divide pivot row has little parallelism
- OK on machines with excess memory bandwidth, but
- Too much data movement per step

1984 - 1990

- “Attack of the Killer Micros”, Brooks @ SC90
- Cache based & SMP machines
- Blocked partitioned algorithms was the way to go
  - Reduce data movement; today’s buzzword “Communication avoiding”
- Level 2 BLAS standard published (mat-vec ops)
- Level 3 BLAS standardization started (mat-mat ops)





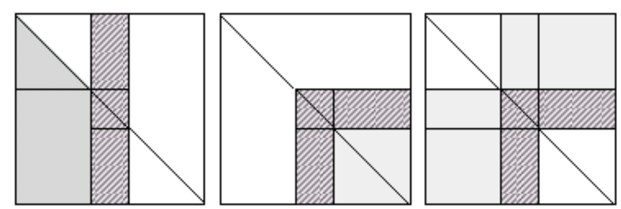


Factor panel (Level 1,2 BLAS)

Triangular Update (Level 3 BLAS)

Schur complement update (Level 3 BLAS)

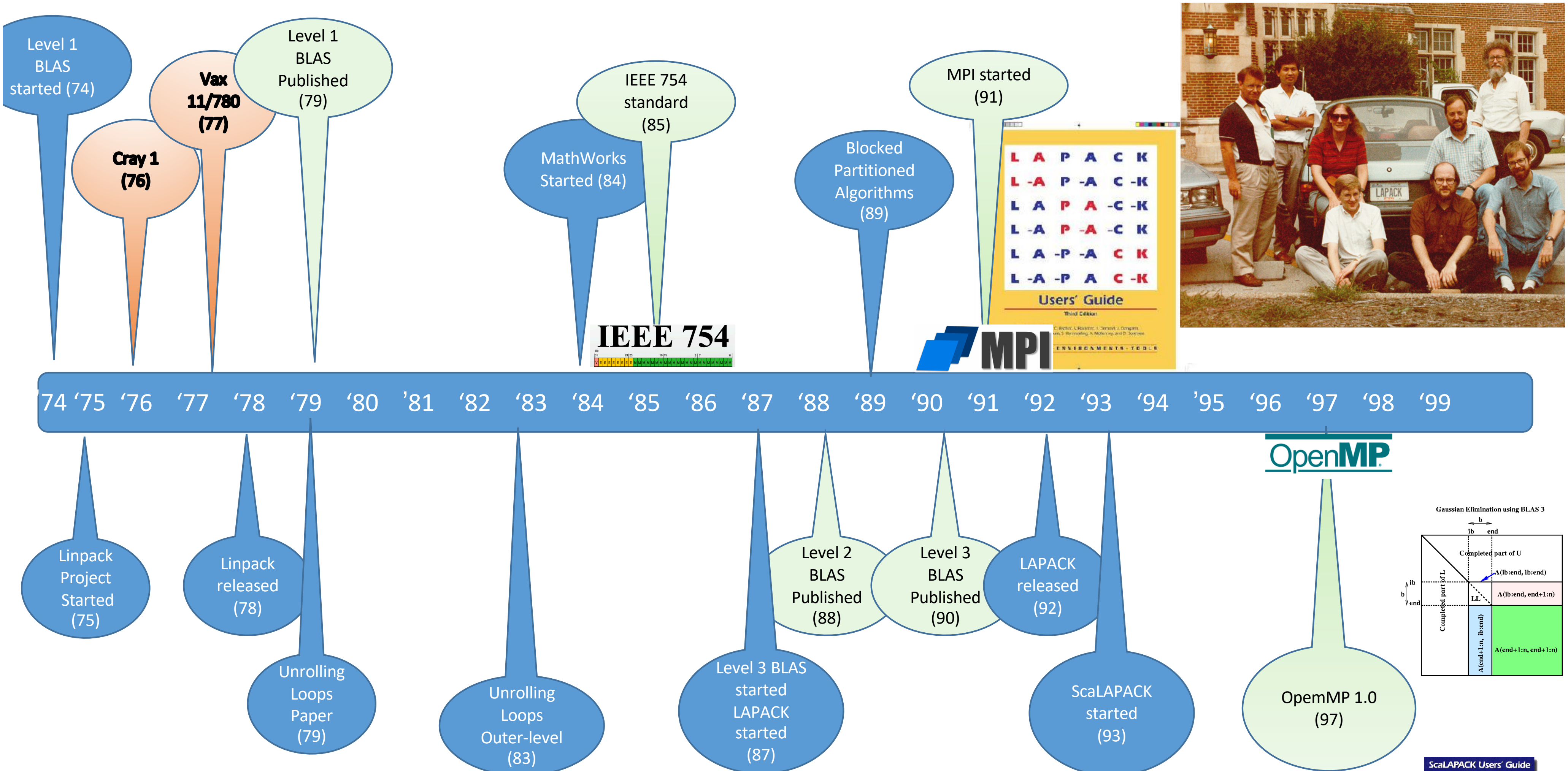
Next Step



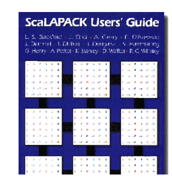
Left-looking LU

Right-looking LU

Crout LU



- LAPACK Published
- ScaLAPACK started



LAPACK Software

Jointly with UTK and UCB and Many Other Contributors

- First release in February 1992
- Current: LAPACK Version 3.9.0 (Nov, 2019) ~2M LoC
- **LICENSE**: Mod-BSD, freely-available software package - Thus, it can be included in commercial software packages (and has been). We only ask that proper credit be given to the authors.
- Public GitHub repository
- **4 Precisions:** single, double, complex, double complex
  - *Considering 16-bit floating point version*
- **Multi-OS** *nix, macOS, Windows
- **Multi-build** support (Make and Cmake)
- **Reference BLAS and CBLAS**
- **LAPACKE: Standard C language APIs for LAPACK**
- Prebuilt Libraries for **Windows**
- Extensive test suite
- **Forum and User support:** http://icl.cs.utk.edu/lapack-forum/
- Goal: bug free library – Since 2009, 165 bugs reported, only 11 pending correction

LAPACK Functionality

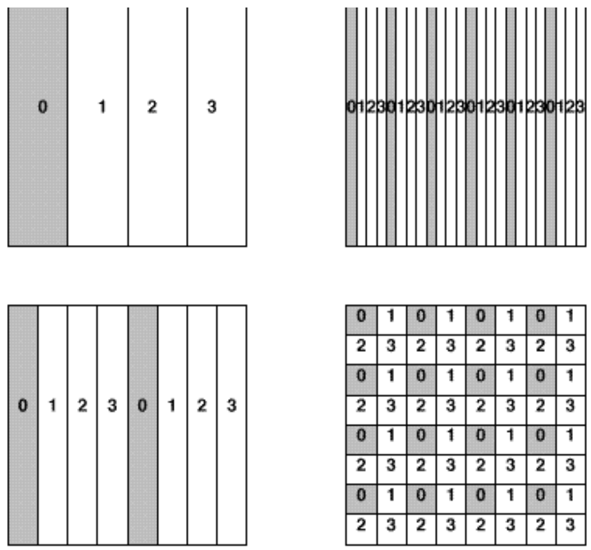
Type of Problem	Acronyms
Linear systems of equations	SV
Linear least squares problems	LS
Linear equality-constrained least squares problems	LSE
General linear model problem	GLM
Symmetric eigenproblems	EV
Nonsymmetric eigenproblems	EV
Singular value decomposition	SVD
Generalized symmetric definite eigenproblems	GV
Generalized nonsymmetric eigenproblems	GG
Generalized (or quotient) singular value decomposition	GG

ScaLAPACK

- Library of software dealing with dense & banded routines
- Distributed Memory - Message Passing
  - When project started MPI didn't exist
- MIMD Computers and Networks of Workstations, Clusters of SMPs
- Data layout critical for performance

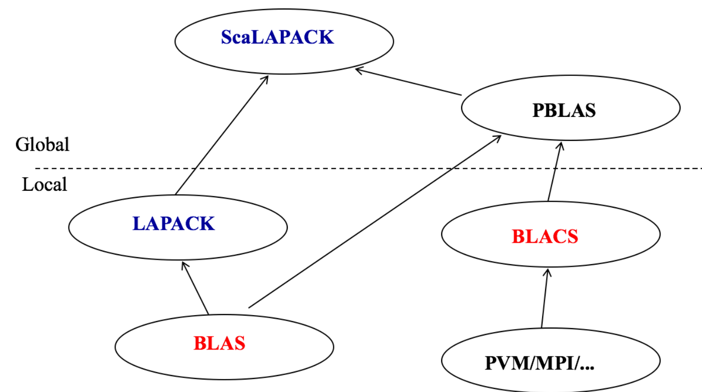
♦ Relies on LAPACK / BLAS and BLACS / MPI

♦ Includes PBLAS (Parallel BLAS)



ScaLAPACK Programming Style

- SPMD Fortran 77 using an object based design
- Built on various modules
  - PBLAS Interprocessor communication & computation
    - BLAS
    - BLACS
      - Targeted PVM, IBM SP, CRI T3, Intel, TMC
        - MPI when standardized
      - Provides right level of abstraction.
- Object based - Array descriptor
  - Contains information required to establish mapping between a global array entry and its corresponding process and memory location.
  - Provides a flexible framework to easily specify additional data distributions or matrix types.
  - Currently dense, banded, & out-of-core
- Using the concept of context



Performance Issues with ScaLAPACK

- The major problem with ScaLAPACK is the lack of overlap of computation and communication .
  - No overlap, resulting in performance issues
- Each phase done separately, bulk synchronous.
  - Computation phase then a communication phase.
  - All (most) processes compute then a communication phase (broadcast)
  - This is how the PBLAS operate.

- Need a "new" interface which allows computation and communication to take place simultaneously, in an asynchronous fashion.

OpenMP in LAPACK and ScaLAPACK

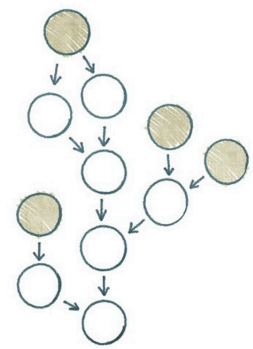
- LAPACK and ScaLAPACK, in general, don't use OpenMP directly, just in the BLAS kernels
  - So to some extent the BLAS may be implemented using OpenMP
- There is an exception – one of the newer routines
  - 2-stage eigenvalue routines for the bulge chasing.
  - LAPACK has OpenMP in the "bulge chasing" stage
  - for 2-stage symmetric and hermitian eigensolver.
- The routines are:
  - real: {s,d}sytrd_sb2st
  - complex: {c,z}hetrd_hb2st
- It uses tasking.
  - If tasks were not used then only a single core cache would be used.
  - With tasks, the caches are combined and data reuse increases.
- And all of this is in Fortran.

Since LAPACK and ScaLAPACK

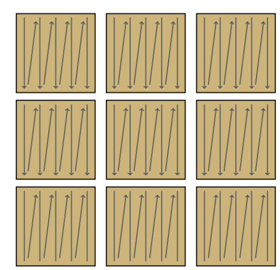
- A lot has changed
  - OpenMP
  - Manycore and accelerators
  - Use a different set of ideas to provide efficient use of underlying hardware
    - PLASMA/DPLASMA
    - MAGMA

PLASMA

- PLASMA is a dense linear algebra library
  - For shared-memory multi-core processors.
  - Algorithms are expressed as sequential kernels acting on tiles of data
  - Runtime takes sequential kernels (tasks), uses task-superscalar scheduling, and exposes parallelism
- Linear algebra for OpenMP
  - dataflow scheduling
  - tile matrix layout
  - tile algorithms



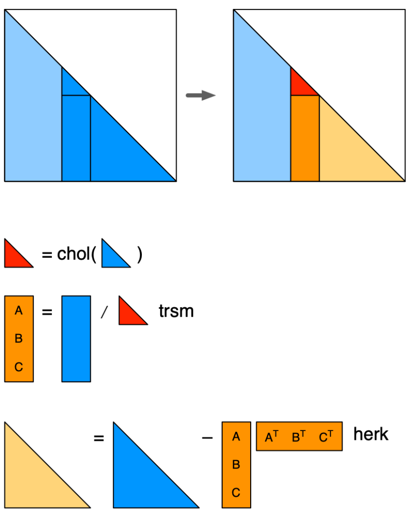
Tile Layout



A. Buttari, J. Langou, J. Kurzak, J. Dongarra,
A class of parallel tiled linear algebra algorithms for multicore architectures,
Parallel Computing, 35(1):38-53, 2009.
DOI: 10.1016/j.parco.2008.10.002

Tile Algorithms

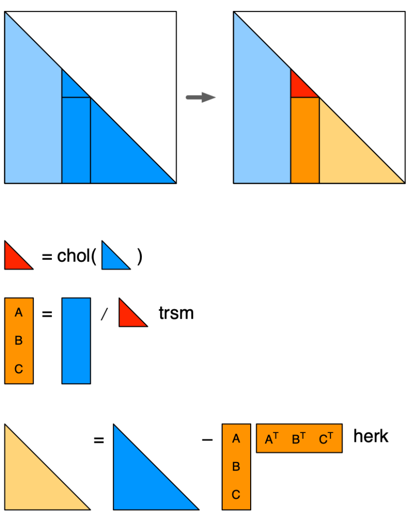
LAPACK Algorithm



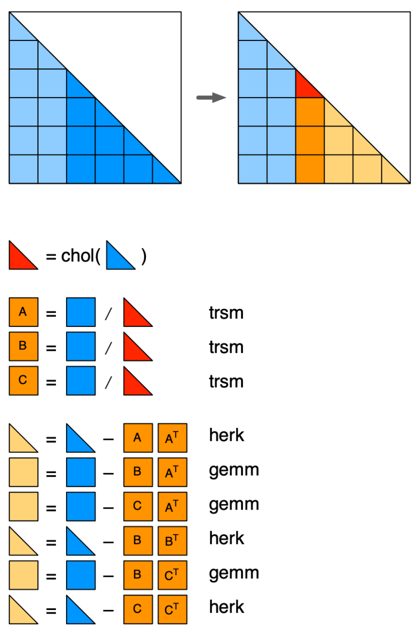
Tile Algorithms

- Decompose large operations into many small operations on tiles
- Track dependencies between tiles
- Parallelism implicit in task graph

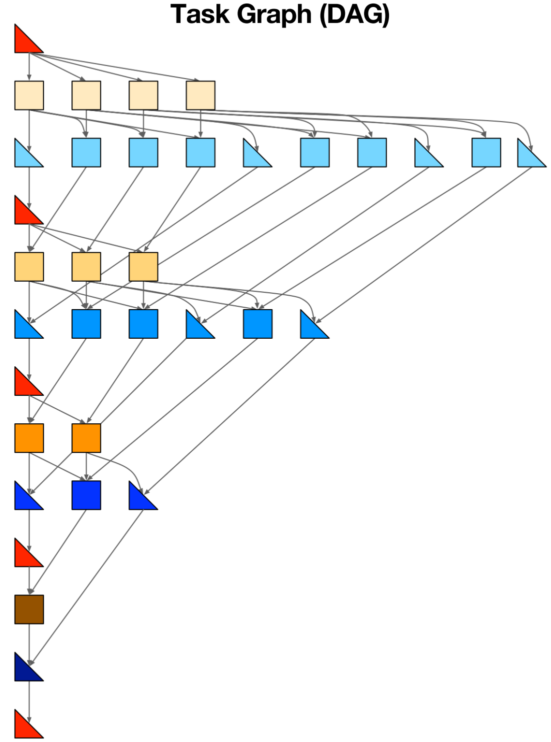
LAPACK Algorithm



Tile Algorithm

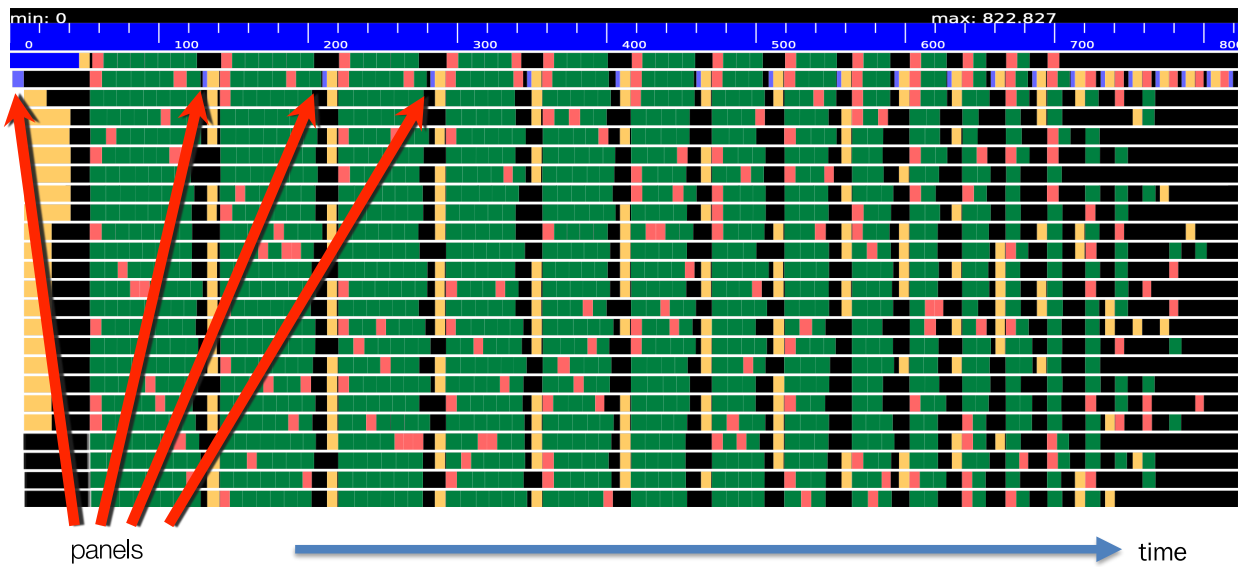


Task Graph (DAG)



Execution trace

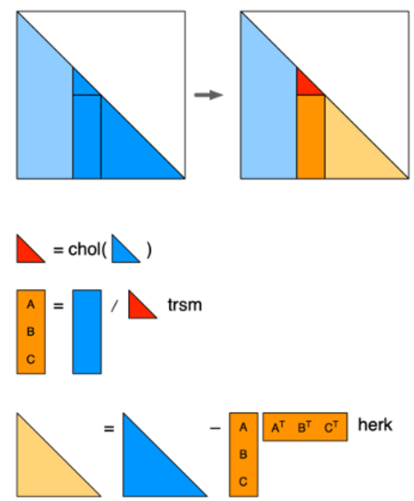
- LAPACK-style fork-join leave cores idle



24 cores
Matrix is 8000 x 8000, tile size is 400 x 400.

potrf trsm syrk gemm idle

LAPACK Algorithm



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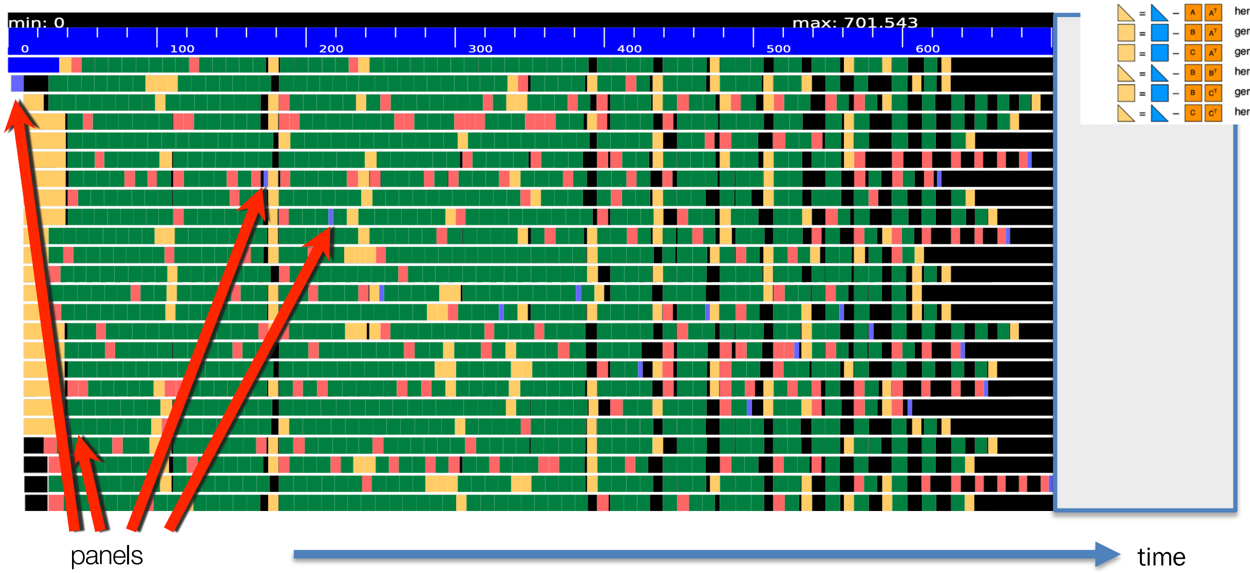
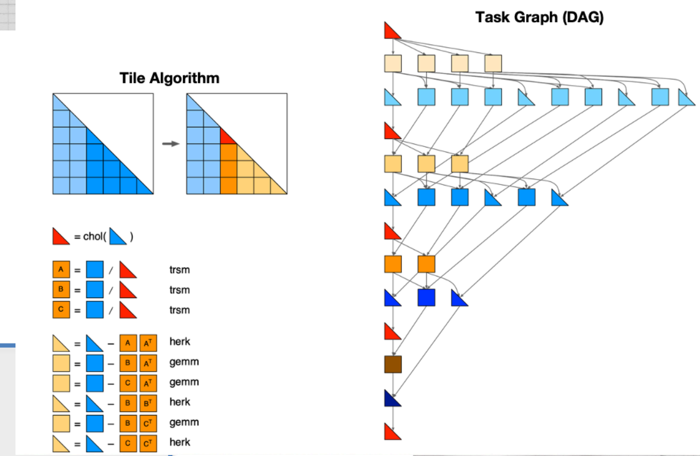
Execution trace

- PLASMA squeezes out idle time



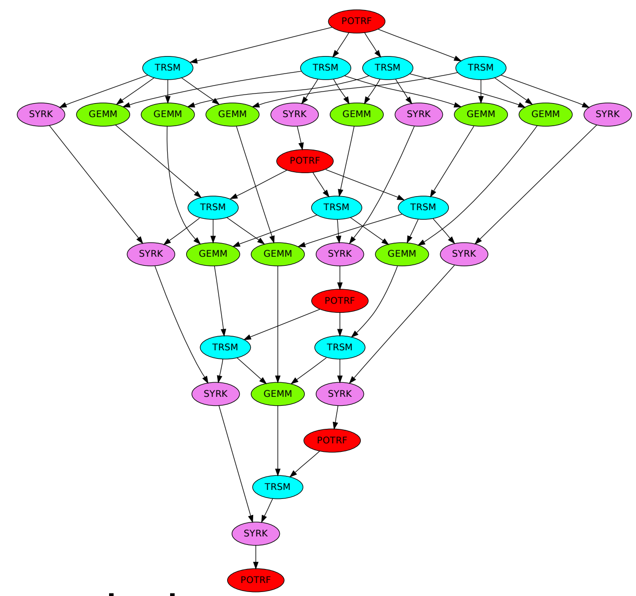


24 cores
Matrix is 8000 x 8000, tile size is 400 x 400.

potrf trsm syrk gemm idle

QUARK Runtime system for PLASMA

- PLASMA needed a way to express the DAGs
- Initial dataflow execution engine in PLASMA
  - For each task inserted, data is marked R, W, RW
  - Future tasks accessing data create a dependency
  - The dependencies form an implicit task-DAG
- QUARK uses superscalar execution
  - Creates a list of tasks and data accessed
  - Tracks data dependencies
  - Launches out-of-order parallel task execution
  - Uses a window of active tasks to limit memory usage
- QUARK allows task-priorities, task-locality, multi-threaded tasks, task-sequence cancellation, incremental runtime-dependencies and other execution ideas…



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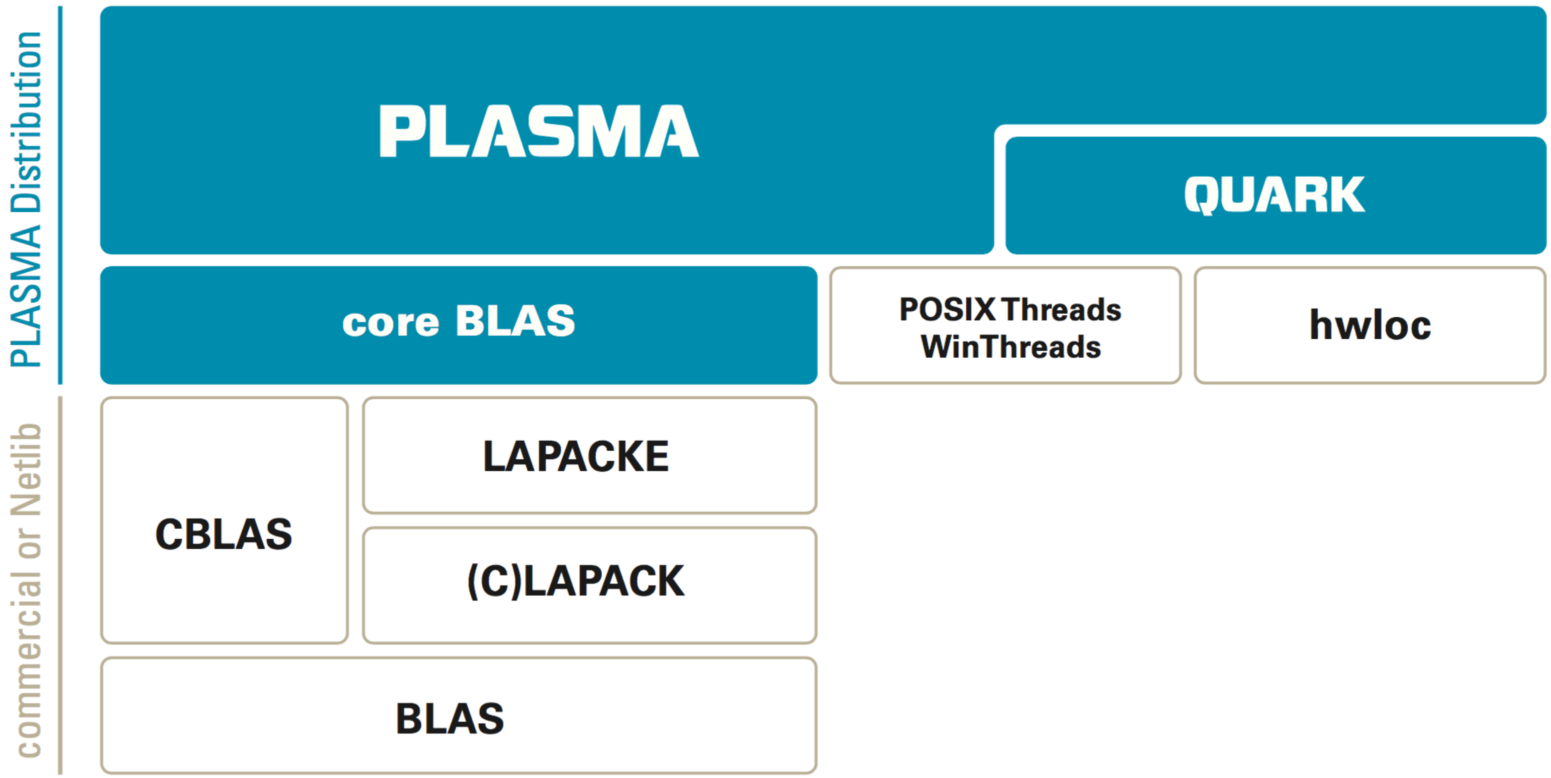
PLASMA: Original Design (Discontinued with Version 2.8)



Dynamic Scheduling, OpenMP, GNU GCC

May 2008	OpenMP 3.0	
April 2009		GCC 4.4
July 2013	OpenMP 4.0	
April 2014		GCC 4.9
Nov. 2015	OpenMP 4.5	
April 2016		GCC 6.1
Nov. 2018	OpenMP 5.0	
May 2019		GCC 9.1
Nov. 2019	OpenMP 5.1 preview	

```
#pragma omp task

#pragma omp task depend

#pragma omp task priority

#pragma omp task affinity(A)
                 detach(hndl)
```

PLASMA: From QUARK to OpenMP

- OpenMP 4.0 adopted task superscalar scheduling (2013)
  - OpenMP 4.5 added task priorities (2015)
- QUARK was phased out in favor of the standard OpenMP runtime
  - Compiler support removed the need to pack/unpack arguments
  - All this:

```
QUARK_Insert_Task(
    quark, CORE_dpotrf_quark, task_flags,
    sizeof(PLASMA_enum),       &uplo,     VALUE,
    sizeof(int),               &n,        VALUE,
    sizeof(double)*nb*nb,       A,        INOUT,
    sizeof(int),               &lda,      VALUE,
    sizeof(PLASMA_sequence*),  &sequence, VALUE,
    sizeof(PLASMA_request*),   &request,  VALUE,
    sizeof(int),               &iinfo,    VALUE,
    0);
```

```
void CORE_dpotrf_quark(Quark *quark)
{
    PLASMA_enum uplo;
    int n;
    double *A;
    int lda;
    PLASMA_sequence *sequence;
    PLASMA_request *request;
    int iinfo;

    int info;
    quark_unpack_args_7(quark, uplo, n, A, lda, sequence, request, iinfo);
    info = LAPACKE_dpotrf_work(
        LAPACK_COL_MAJOR,
        lapack_const(uplo),
        n, A, lda);
    if (sequence->status == PLASMA_SUCCESS && info != 0)
        plasma_sequence_flush(quark, sequence, request, iinfo+info);
}
```

  - Replaced by this:

```
#pragma omp task depend(inout:A(k, k)[0:nb*nb])
LAPACKE_dpotrf_work(
    LAPACK_COL_MAJOR,
    'L', nb, A(k, k), nb);
```

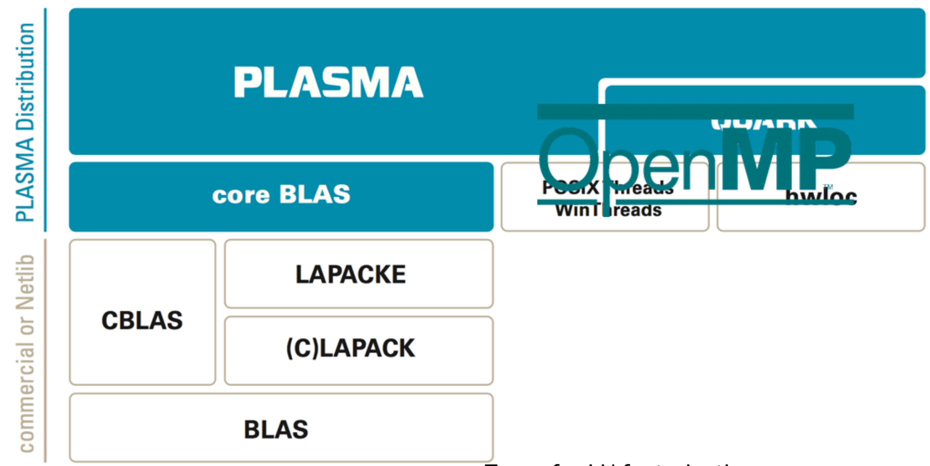
PLASMA: From QUARK to OpenMP

- PLASMA tile algorithms map well from QUARK to OpenMP
  - QUARK task insertion maps directly to OpenMP task pragmas
- Task priorities allow tasks on the critical path to be prioritized
  - Tile algorithm tasks are sequentially presented to the runtime
  - Critical path tasks may not be exposed to the runtime early
  - Algorithms need to present-unroll tasks in the right order
- A few features are require attention to match with OpenMP, i.e…
  - QUARK has thread-data-affinity hinting, now in OpenMP 5
  - QUARK has multi-threaded tasks often called gang-tasks;
    - These are tasks that take multiple-threads which all work on a common activity like the panel.
  - QUARK tasks can be locked to threads or thread-masks (set of threads)

YarKhan, A., Kurzak, J., Luszczek, P., & Dongarra, J. (2016). Porting the PLASMA numerical library to the OpenMP standard. *International Journal of Parallel Programming*, *45*(3), 612-633.

PLASMA with OpenMP

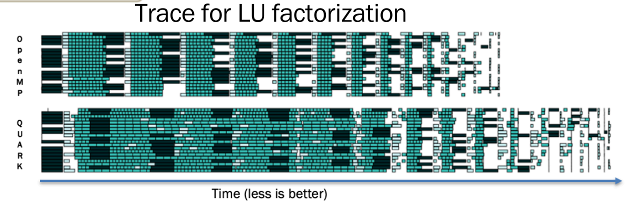
- PLASMA version 17 switched to OpenMP
  - Transition led to redesigning some algorithms; notably LU factorization
- OpenMP is supported by industry and community
  - Optimized implementations
  - New features (e.g. target offload to accelerators)
  - High adoption in HPC community
  - Allows interoperability with other OpenMP software



A. YarKhan, J. Kurzak, P. Luszczek, J. Dongarra, Porting the PLASMA Numerical Library to the OpenMP Standard, International Journal of Parallel Programming, pp. 1-22, 2016. DOI: 10.1007/s10766-016-0441-6

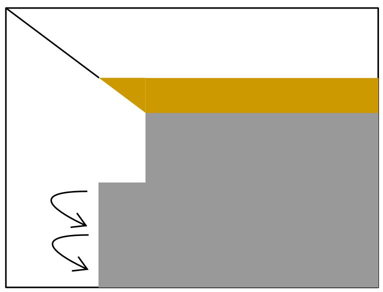
Dongarra, J., Gates, M., Haidar, A., Kurzak, J., Luszczek, P., Wu, P., Yamazaki, I., YarKhan, A., Abalenkovs, M., Bagherpour, N. and Hammarling, S., 2019. PLASMA: Parallel linear algebra software for multicore using OpenMP. *ACM Transactions on Mathematical Software (TOMS)*, *45*(2), pp.1-35.

Trace for LU factorization

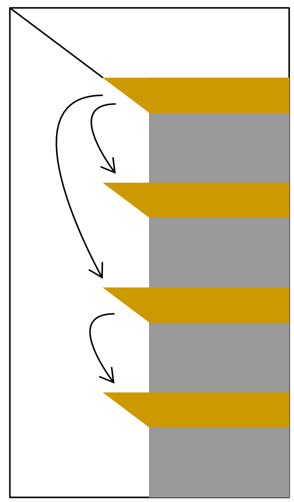


Tiles are of size 288 × 288 elements.
The matrix is of size 15 × 15 tiles.
The system consists of 20 Intel Haswell cores

PLASMA – QR Factorization



Tile QR
(incremental)



TSQR / CAQR
(tree reduction)

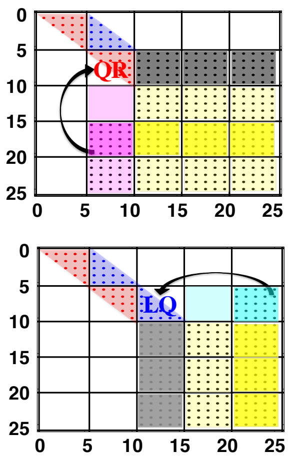
<u>Tile QR</u>

- great for square matrices
- great for multicore processors

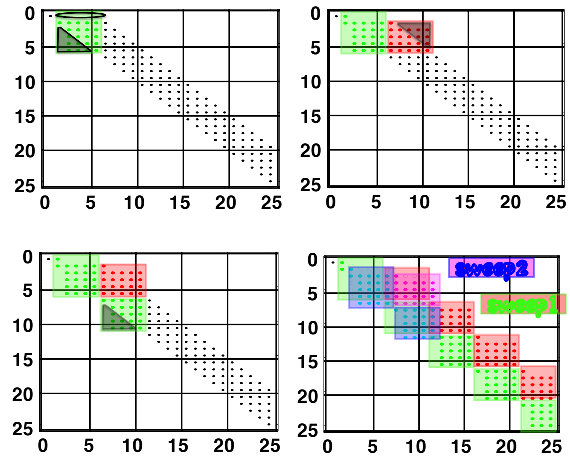
<u>TSQR / CAQR</u>

- great for tall and skinny matrices
- great for distributed memory

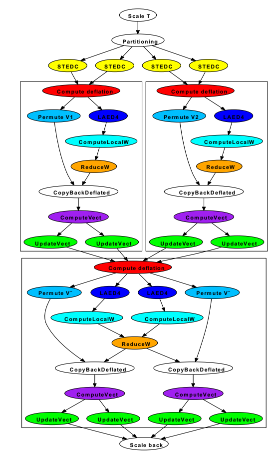
PLASMA – Algorithms – SVD/EVP (symmetric)



reduction to band
parallel & cache efficient
tile algorithm



band reduction
parallel & cache efficient
a flavor of communication avoiding

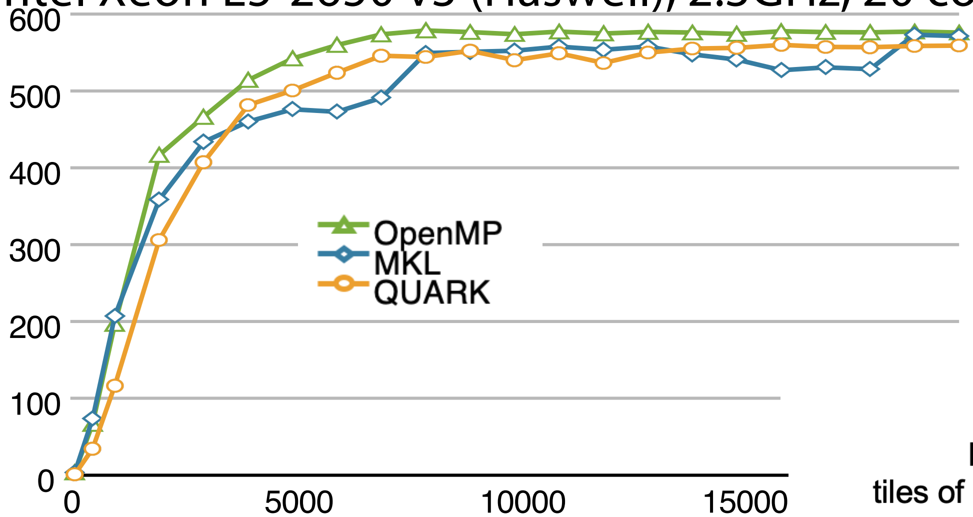


divide and conquer
task-based
dataflow

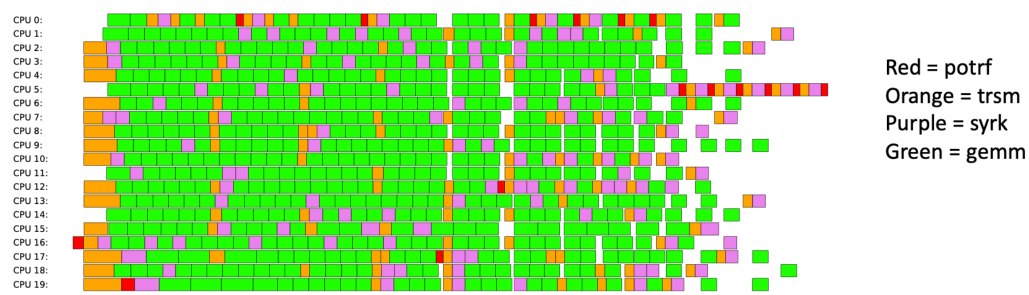
PLASMA OpenMP Cholesky Performance

double precision Cholesky factorization

Intel Xeon E5-2650 v3 (Haswell), 2.3GHz, 20 cores

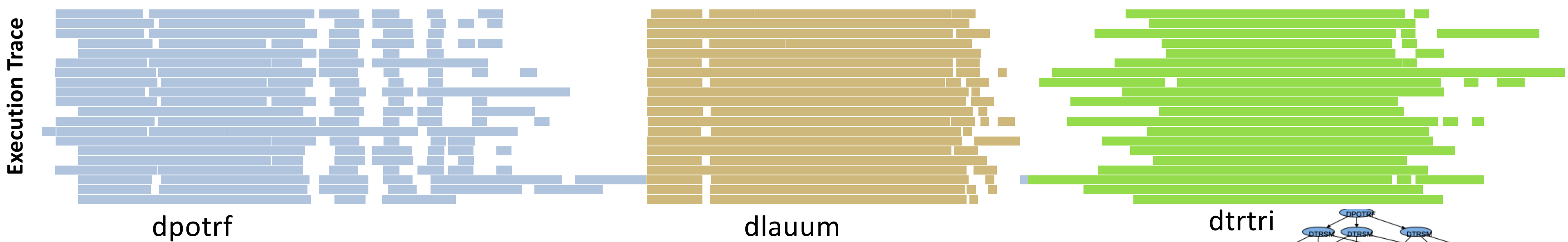


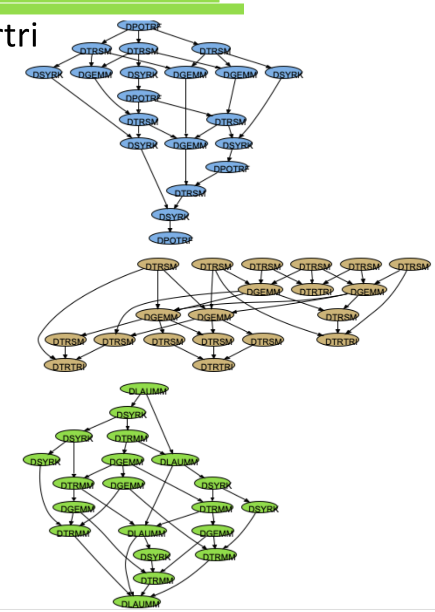
PLASMA Cholesky factorization using OpenMP
Intel Xeon E5-2650 v3 (Haswell) 2.3GHz 20 cores
tiles of size 224 x 224, matrix of size 20 x 20 tiles (4480 x 4480)



PLASMA OpenMP Cholesky Inversion Trace

PLASMA Cholesky inversion using OpenMP
Intel Xeon E5-2650 v3 (Haswell) 2.3GHz 20 cores
tiles of size 224 x 224, matrix of size 13 x 13 tiles (2912 x 2912)





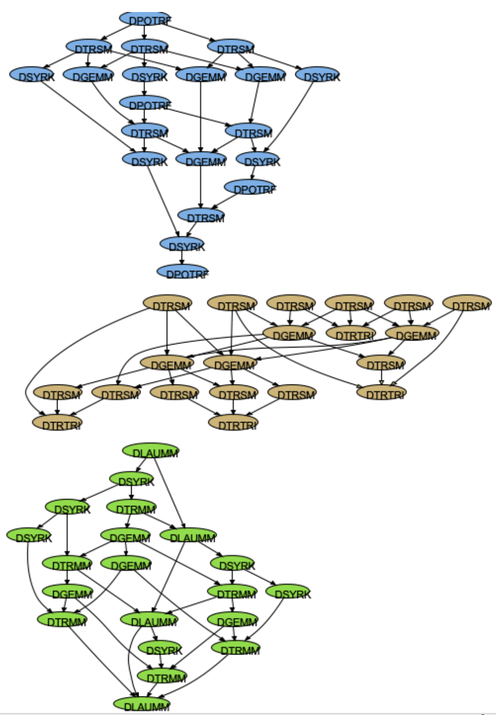
```
plasma_dpotrf(uplo, n, pA, lda);
plasma_dlauum(uplo, n, pA, lda);
plasma_dtrtri(uplo, diag, n, pA, lda);
```

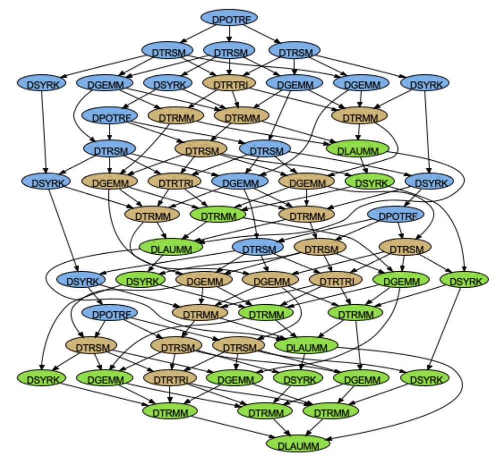
PLASMA OpenMP Cholesky Inversion Code

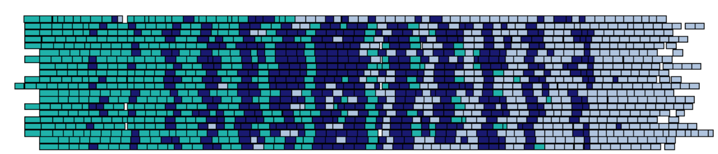
```
#pragma omp parallel
#pragma omp master
{
    plasma_omp_zge2desc(pA, lda, A, sequence, &request);

    plasma_omp_dpotrf(uplo, A, sequence, &request);
    plasma_omp_zlauum(uplo, A, sequence, &request);
    plasma_omp_ztrtri(uplo, diag, A, sequence, &request);

    plasma_omp_zdesc2ge(A, pA, lda, sequence, &request);
}
```

PLASMA OpenMP Cholesky Inversion DAG

PLASMA Cholesky inversion using OpenMP
Intel Xeon E5-2650 v3 (Haswell) 2.3GHz 20 cores
tiles of size 224 x 224, matrix of size 13 x 13 tiles (2912 x 2912)



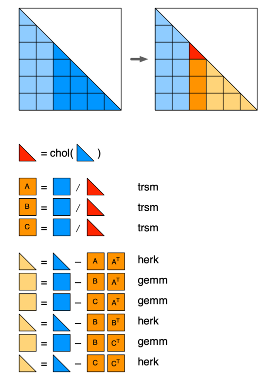


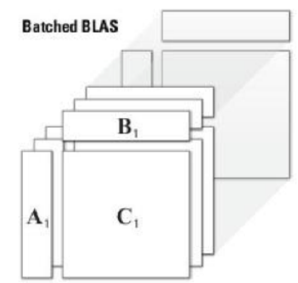


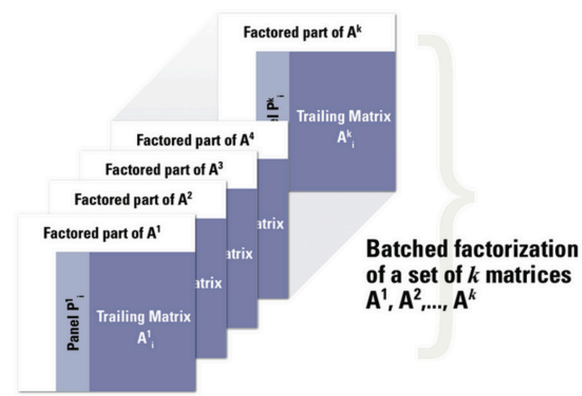
Standard for Batched Computations

- Define standard API for batched BLAS and LAPACK in collaboration with Intel/Nvidia/other users
- Fixed size: most of BLAS and LAPACK released
- Variable size: most of BLAS released
- Variable size: LAPACK in the branch
- Native GPU algorithms (Cholesky, LU, QR) in the branch
- Tiled algorithm using batched routines on tile or LAPACK data layout in the branch

- Framework for Deep Neural Network kernels
- CPU, KNL and GPU routines
- FP16 routines in progress

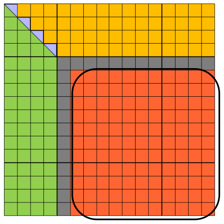




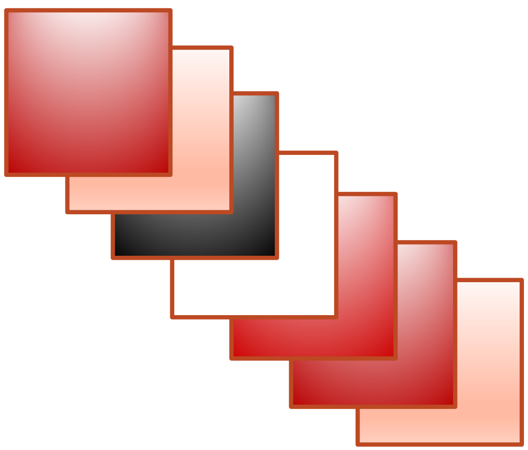


Batched Computations

- **Non-batched computation**
- **loop over the matrices one by one** and compute using multithread (note that, since matrices are of small sizes there is not enough work for all the cores). So we expect low performance as well as threads contention might also affect the performance

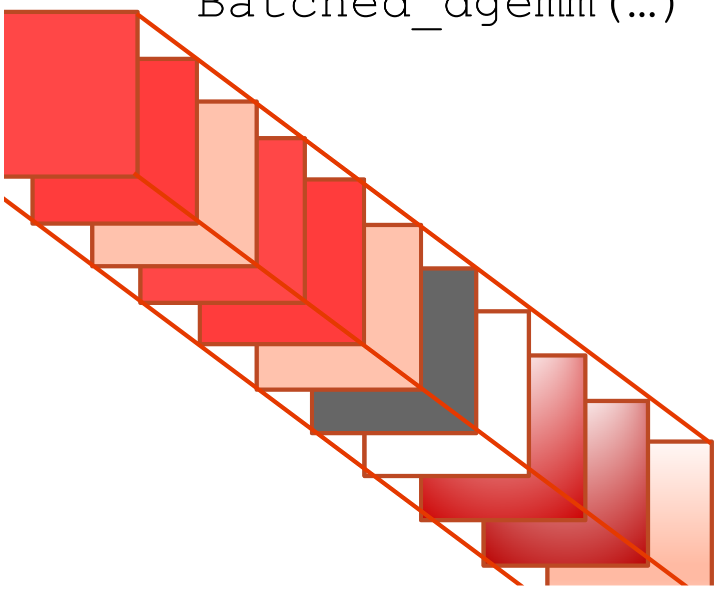


```
for (i=0; i<batchcount; i++)
   dgemm(…)
```

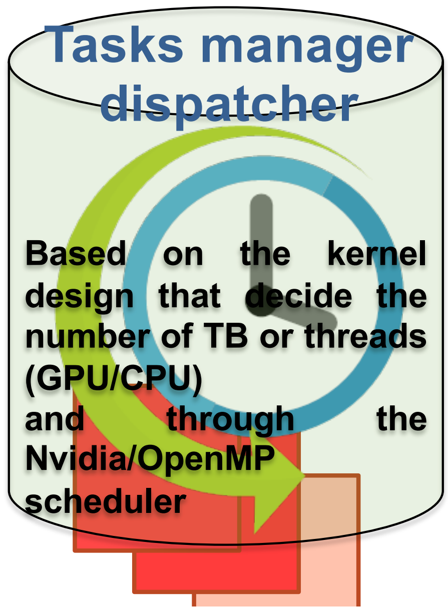


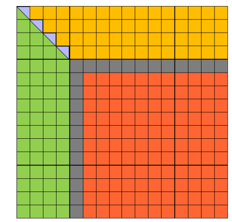
Batched Computations

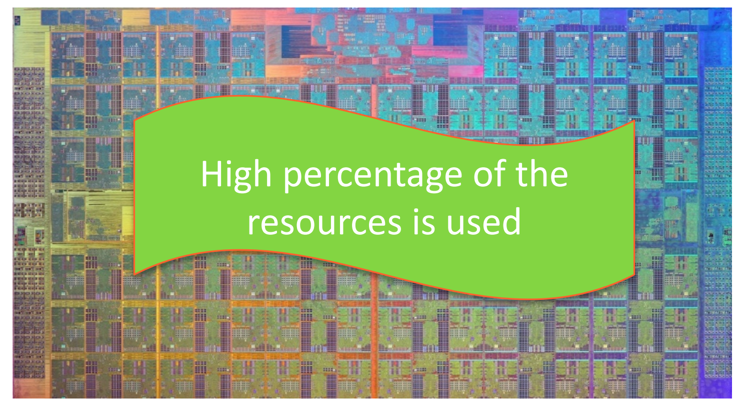
- **Batched computation**
- **Distribute all the matrices over the available resources by assigning a matrix to each group of core/TB to operate on it independently**
  - For very small matrices, assign a matrix/core (CPU) or per TB for GPU
  - For medium size a matrix go to a team of cores (CPU) or many TB’s (GPU)
  - For large size switch to multithreads classical 1 matrix per round.



`Batched_dgemm(…)`

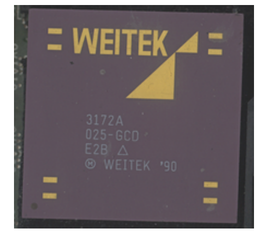






Accelerators to Enhance Performance
We Have Seen This Before

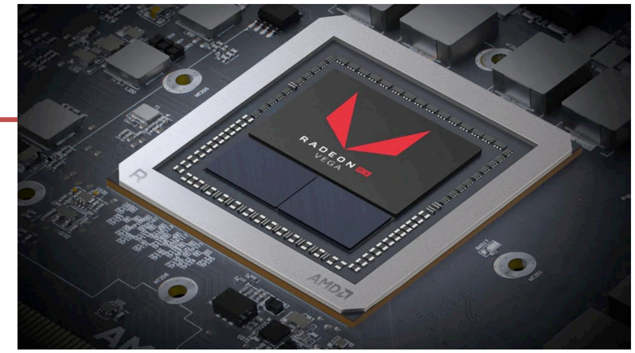
- Floating Point Systems FPS-164/MAX Supercomputer (1976)
- Intel Math Co-processor (1980)
- Weitek Math Co-processor (1981)



1976

1980

Today Many HPC Systems …



- Use a hybrid architecture design
  - Think standard multicore chips and accelerators (GPUs)
- Successive generations become more integrated
- AMD's Radeon Instinct Mi100 GPU
- Nvidia's Ampere GPU
- Intel's Xe Ponte Vecchio GPU

Data Center GPU Name	NVIDIA Tesla V100	NVIDIA A100
GPU Codename	GV100	GA100
GPU Architecture	NVIDIA Volta	NVIDIA Ampere
SMs	80	108
GPU Boost Clock	1530 MHz	1410 MHz
Peak FP16 Tensor Core TFLOPS[1]	125	312
Peak Bfloat16 Tensor Core TFLOPS[1]	NA	312
Peak TF32 Tensor TFLOPS[1]	NA	156
Peak FP64 Tensor TFLOPS[1]	**NA**	**19.5**
Peak INT8 Tensor TOPS[1]	NA	624
Peak FP16 TFLOPS[1]	31.4	78
Peak Bfloat16 TFLOPS[1]	NA	39
Peak FP32 TFLOPS[1]	15.7	19.5
Peak FP64 TFLOPS[1]	7.8	9.7
Peak INT32 TOPS[1]	15.7	19.5
Memory Interface	4096-bit HBM2	5120-bit HBM2
Memory Size	32 GB / 16 GB	40 GB
Memory Data Rate	877.5 MHz DDR	1215 MHz DDR
Memory Bandwidth	900 GB/sec	1.6 TB/sec
L2 Cache Size	6144 KB	40960 KB
Shared Memory Size / SM 1.Peak rates are based on GPU Boost Clock	Configurable up to 96 KB	Configurable up to 164 KB

MAGMA

Provides highly optimized LA for GPUs
Designed for single node with multiple GPUs
Research vehicle for LA on new architectures

for architectures in
{ CPUs + Nvidia GPUs (**CUDA**),
CPUs + AMD GPUs (**HIP** & **OpenCL**),
CPUs + Intel Xeon Phis,
manycore (native: GPU or **KNL**/CPU),
embedded systems, combinations
}

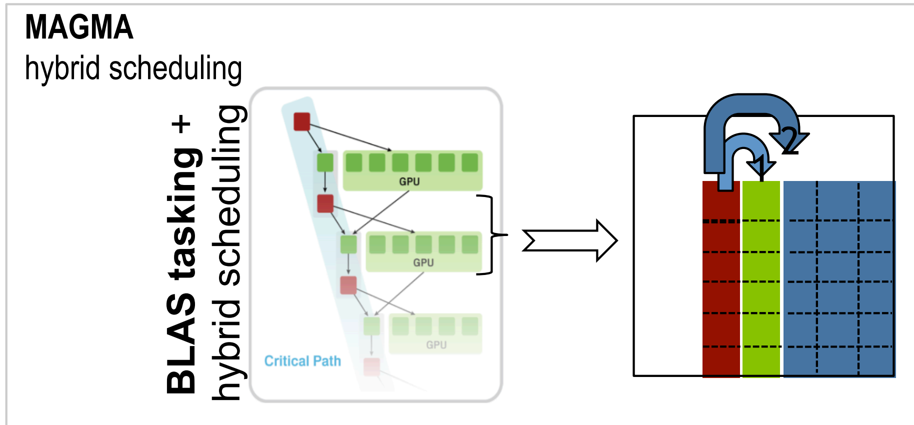
for precisions in
{ s, d, c, z,
half-precision (FP16),
mixed, … }

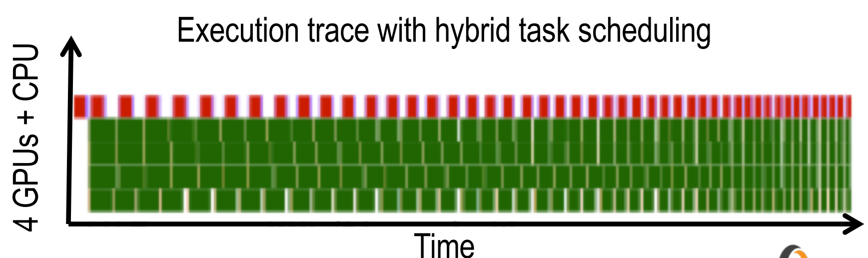
for interfaces
{ heterogeneous CPU/GPU, native, … }

- **LAPACK**
- **BLAS**
- **Batched LAPACK**
- **Batched BLAS**
- **Sparse**
- **Tensors**
- **MAGMA-DNN**
- **Templates**
- …

How to design for performance and energy efficiency

Programming model: BLAS tasks + scheduling





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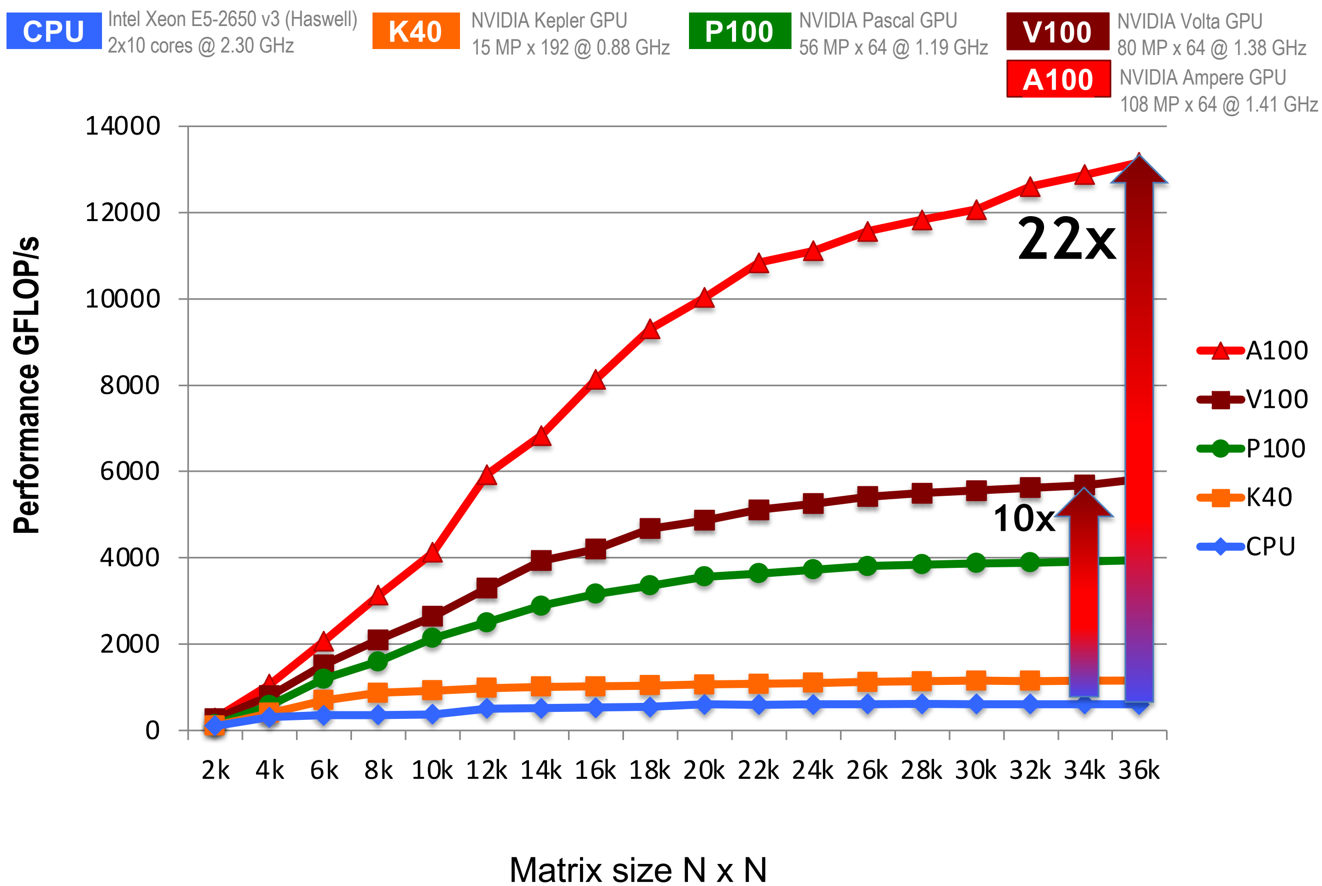
MAGMA on Nvidia GPUs

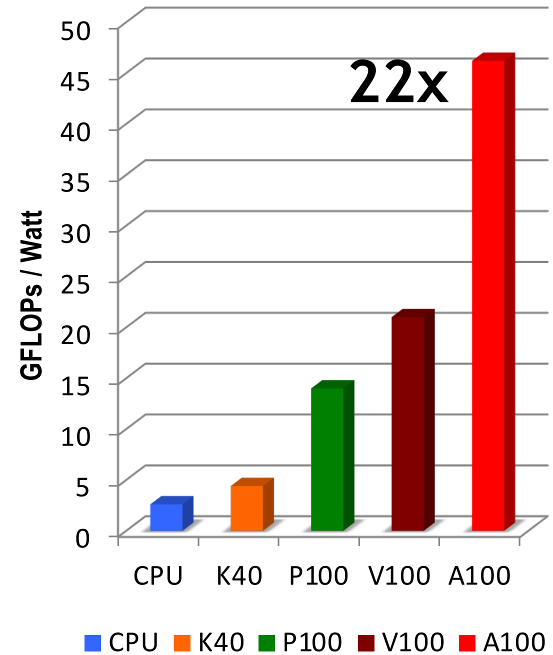
PERFORMANCE & ENERGY EFFICIENCY

MAGMA 2.5.3 LU factorization in double precision arithmetic



Energy efficiency

(under ~ the same power draw)



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Scheduling of computational tasks

- **Main scheduling mechanism in MAGMA is data flow driven using streams**
- **MAGMA research has explored use of OpenMP scheduling (similar to approach in PLASMA)**

J. Dongarra, A. Haidar, O. Hernandez, S. Tomov, M. Venkata,
"**POMPEI: Programming with OpenMP4 for Exascale Investigations**",
ICL Technical report, December, 2017.

Other uses of OpenMP in MAGMA

- **Batched LA on CPUs uses OpenMP**
- **Divide & Conquer for Hermitian or real symmetric matrices use OpenMP (in a hybrid algorithm that runs Divide & Conquer on the CPU)**
- **MAGMA Sparse uses OpenMP in incomplete LU; data-format preparations, transformations, and initializations, etc.**

Department of Energy's Exascale Computing Project (ECP)

- As part of DOE's ECP we are working on a package to fit within the architectures for Exascale systems.
- The research within LAPACK, ScaLAPACK, PLASMA and MAGMA will go into a new package called SLATE
    - Software for Linear Algebra Targeting Exascale

Software for Linear Algebra Targeting Exascale (SLATE)

Focused on Dense Linear Algebra Problems

- Linear systems of equations $Ax = b$
- Linear least squares $\min \| b - Ax \|_2$
- Singular value decomposition (SVD) $A = U\Sigma V^T$
- Eigenvalue value problems (EVP) $Ax = \lambda x$

- Dense (square, rectangular)
- Band

SLATE's Goals

Target modern HPC hardware

- Multicore processors, multiple accelerators per node

Achieve portable high performance

- Rely on MPI, OpenMP, vendor-optimized BLAS, LAPACK

Scalability

- 2D block cyclic distribution, arbitrary distribution, dynamic scheduling, communication overlapping

Assure maintainability

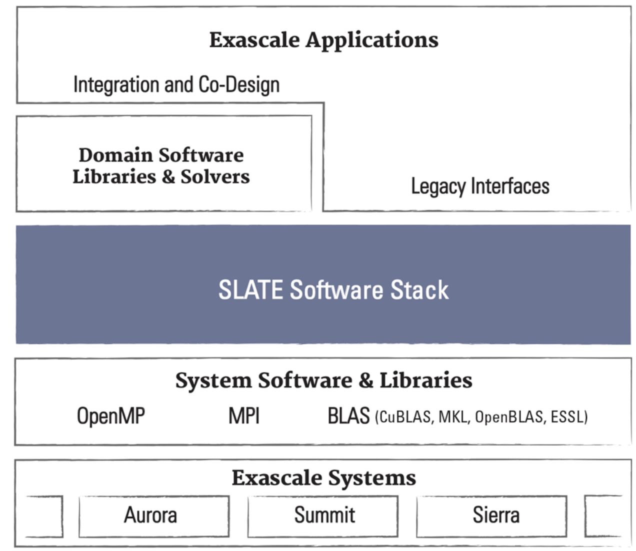
- C++ templating and other features to minimize codebase

Ease transition from ScaLAPACK

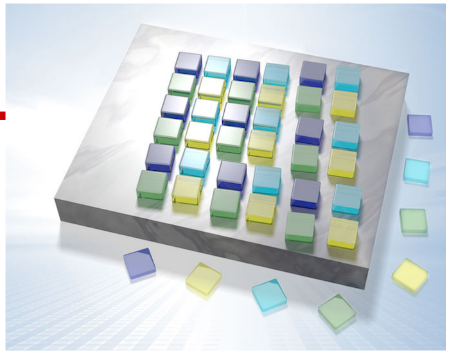
- Natively support ScaLAPACK 2D block-cyclic layout, backwards compatible API

Flexibility

- Users can construct new routines from well-designed parts



SLATE design



- Modern C++ replacement for ScaLAPACK
  - Code templated for precision
  - Backwards compatibility layer
- Flexible
  - Non-uniform block sizes
  - Arbitrary distributions; default 2D block-cyclic
- Standards based
  - MPI for distributed communication
  - OpenMP 4.5 tasks for shared memory parallelism
  - Includes GPU support, currently using cuBLAS
  - S,D,C,Z,H (float16) precisions
- Developed from scratch as ECP project
- LAPACK/ScaLAPACK calling sequences mapping to SLATE

SLATE: Abstraction Layer

programing frameworks

Leverage emerging programming frameworks for scheduling tasks to large scale machines with multicores, accelerators and complex memory systems.
Perhaps plug into different run-time systems

- Runtime provides …
  - Dynamic task scheduling
    - Mutithreading
    - Accelerator offload
  - Accelerator memory management
    - Basically a cache model with LRU policy
  - Communication hiding
    - Asynchronous message passing
    - Asynchronous PCI DMAs (host-device)
- Investigating PaRSEC (UTK), StarPU (INRIA), Kokkos (SNL), Legion (Stanford),…

Coverage

Basic linear algebra $(C = AB, \ldots)$

	ScaLAPACK	SLATE
Level 1 PBLAS	✔	✘ (use Level 3)
Level 2 PBLAS	✔	✘(use Level 3)
Level 3 PBLAS	✔	✔
Matrix norms	✔	✔
Test matrix generation	✔	✔ (new)

Least squares $(Ax \cong b)$

	ScaLAPACK	SLATE
QR	✔	✔
LQ	✔	✔ (new)
Least squares solver	✔	✔

Linear systems $(Ax = b)$

	ScaLAPACK	SLATE
LU (partial pivoting)	✔	✔
LU, band (pp)	✔	✔
LU (non-pivoting)	✘	✔ (new)
Cholesky	✔	✔
Cholesky, band	✔	✔ (new)
Symmetric Indefinite (block Aasen)	✘	✔ (CPU only)
Mixed precision (single-double)	✘	✔
Inverses (LU, Cholesky)	✔	✔
Condition estimate	✔	✘

SVD, eigenvalues $(A = U\Sigma V^H, Ax = \lambda x)$

	ScaLAPACK	SLATE
Singular value decomposition (SVD)	✔	✔ values (new)
Symmetric eigenvalues	✔	✔ values (new)
Generalized symmetric eigenvalues	✔	✔ values (new)
Polar decomposition (QDWH)	✘	✔ (new)
Non-symmetric eigenvalues	✘	✘
Hessenberg reduction	✔	2021
Hessenberg eigen solver	• real only	2022
Back-transform	• complex only	2021

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Milestones

- **Completed**
  - Hermitian eigenvalues & SVD — 2-stage reductions ("bulge chasing")
  - Performance improvements (BLAS, norms, Cholesky, QR)
    Developers' Guide
  - Generalized Hermitian eigenvalues
  - Simplified C++ API (`lu_factor` instead of `getrf`)
    C and Fortran APIs
    Users' Guide
- **Upcoming**
  - Performance improvements for LU, Cholesky
  - Port to AMD (HIP) and Intel (oneAPI, OpenMP offload)
  - Performance improvements for QR, eigenvalues, SVD
  - Divide-and-conquer for eigenvalues


SLATE WORKING NOTES 11

SLATE Developers' Guide

Ali Charara
Mark Gates
Jakub Kurzak
Asim YarKhan
Jack Dongarra

Innovative Computing Laboratory

January 8, 2020

SLATE WORKING NOTES 10

SLATE Users' Guide

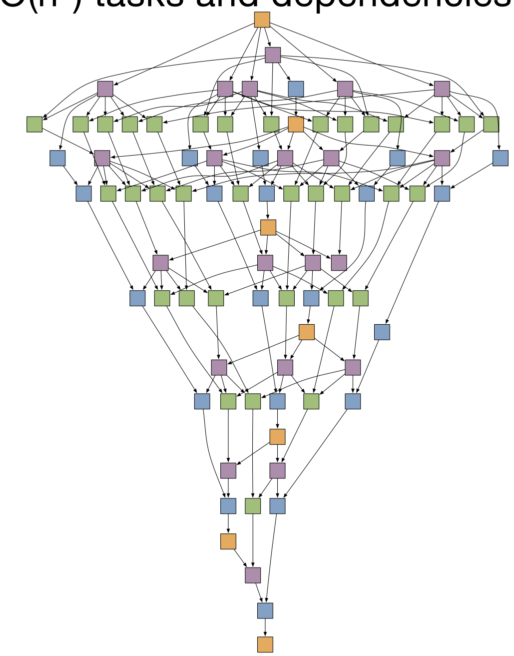
Mark Gates
Ali Charara
Jakub Kurzak
Asim YarKhan
Mohammed Al Farhan
Dalal Sukkari
Jack Dongarra

Innovative Computing Laboratory

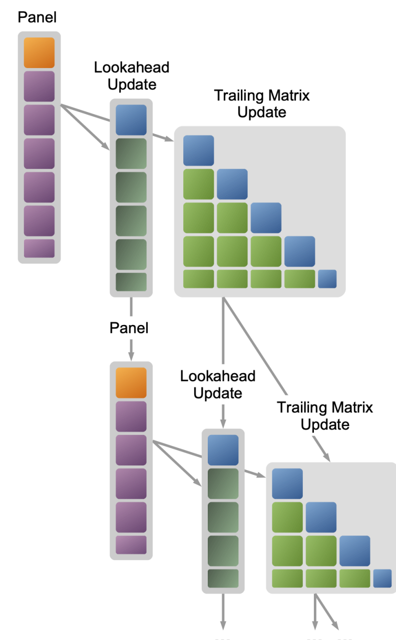
July 7, 2020

Tasks and dependencies

- PLASMA tile-by-tile data flow
  - O(n^3) tasks and dependencies



- SLATE aggregates tiles into large tasks
  - O(n) tasks and dependencies



CPU and GPU Targets

- SLATE algorithms templated for target: CPU Host or GPU Devices
  - One high-level Cholesky code can call different low-level kernels (CPU or GPU)
- Today, user can specify target
- In future, default will be GPU Devices if available, else CPU Host, perhaps based on matrix size

```
// Default on GPU, if available, else CPU.
slate::chol_factor( A );

// User-specified target.
slate::chol_factor( A, {{ Option::Target, Target::Devices }} );
slate::chol_factor( A, {{ Option::Target, Target::Host    }} );
```

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GPU support

- Currently, SLATE directly uses CUDA and cuBLAS
- Plan to add portability layer
  - Support HIP/ROCm, OpenMP offload, or SYCL
  - Primarily rely on vendor BLAS (cuBLAS, hipBLAS, MKL, …)
    - BLAS++ library as portability layer
  - SLATE has few custom kernels to implement in CUDA / HIP / OpenMP offload / SYCL
    - Batched transpose, batched matrix norm, …

SLATE Features

- Runtime interface
  - Use OpenMP
  - Would like to plug into other systems
    - PaRSEC, Legion, Darma, StarPU, …
    - Statically scheduled across nodes; dynamically schedule within node
- Tiled Algorithms
  - Runtime scheduling based on dataflow
  - Runtime dependency tracking
    - Plug into the different runtime systems
- Data distribution as in ScaLAPACK
  - Given the layout and arrangement of processes communication is understood
- Task based parallelism inspired by PLASMA
  - High level DAG enables overlap of computation and communication
- Ability to use accelerators as in MAGMA
  - Hybrid computing using the runtime system

Conclusions

- **Many changes in the past 50 years…**
  - **Hardware, Languages, Standards, Algorithms, and Applications**
- **Standards (both defacto and official) and licensing are important in wide spread adoption of libraries.**
- **As numerical library developers we have tracked the advances and have taken advantage of these changes to enhance the software base.**

50 Years Evolving SW and Algorithm Tracking Hardware Developments

Software/Algorithms follow hardware evolution in time	
EISPACK (1970's) (Translation of Algol to F66)	Rely on - Fortran, but row oriented
LINPACK (1980's) (Vector operations)	Rely on - Level-1 BLAS operations - Column oriented
LAPACK (1990's) (Blocking, cache friendly)	Rely on - Level-3 BLAS operations
ScaLAPACK (2000's) (Distributed Memory)	Rely on - PBLAS Mess Passing
PLASMA & MAGMA (2010's) New Algorithms (many-core friendly & GPU)	Rely on - DAG/scheduler - block data layout - some extra kernels
SLATE (2020's)	Rely on C++ - Tasking DAG scheduling - Tiling, but tiles can come from anywhere - Batched Dispatch